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Research Progress of Graphene Adsorbents in Water Treatment: Mechanism and Function

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ABSTRACT
The problem of global water pollution is becoming increasingly severe and has become a key factor restricting the sustainable development of the ecological environment and the stability of the social economy. Especially, the organic pollutants and heavy metal ions emitted by industries such as chemical and pharmaceuticals, which are difficult to degrade, pose a serious threat to the aquatic ecosystem and human health. Among various water treatment technologies, the adsorption method occupies a core position due to its simple operation, controllable cost, and high removal efficiency. Graphene, as a two-dimensional nanomaterial with an extremely large theoretical specific surface area (2630 m^2/g) and abundant surface functional groups, demonstrates significant advantages in pollutant adsorption due to its unique structural characteristics and has become a hot topic in the research of water treatment adsorption materials. This study focuses on the mechanism of action of graphene adsorbents and their application effects, systematically summarizes the research progress in the field of water treatment, and aims to provide theoretical references for the development of high-performance adsorption materials and their engineering applications. The adsorption performance of graphene adsorbents is closely related to their structural characteristics and surface modification strategies. Graphene oxide, as an important derivative of graphene, can significantly enhance the adsorption capacity for polar pollutants by introducing oxygen-containing functional groups such as hydroxyl and carboxyl. Wu Linlin used chemical and pharmaceutical wastewater as the treatment object and prepared graphene oxide composite materials. The results showed that this material had an adsorption capacity of 187.6 mg/g for antibiotic pollutants in the wastewater, with an removal rate exceeding 92%, and the adsorption process conformed to the quasi-second-order kinetic model.

KEYWORDS
Graphene adsorbent; Water treatment; Adsorption mechanism; Oxidized graphene

1 Introduction

Clarifying the research value of graphene adsorbents and the focus range of the literature review is of great significance for promoting the innovation and development of water treatment technologies. Current research mainly focuses on the preparation process and performance characterization of graphene adsorbents, but a deeper analysis of their adsorption mechanisms (such as the mechanism of interfacial interaction, the matching between functional groups and pollutants) still needs to be enhanced. At the same time, the assessment of their application effects in actual complex wastewater systems is relatively insufficient. This literature review will focus on the mechanistic analysis and application effects of graphene adsorbents, systematically reviewing the influence of structural regulation on adsorption activity, the adsorption mechanisms of typical pollutants, and their treatment performance in simulated and actual wastewater. Wu Linlin used chemical pharmaceutical wastewater as the treatment object and prepared graphene oxide composite materials. The results showed that the adsorption capacity of this material for antibiotic pollutants in the wastewater could reach 187.6 mg/g, with an removal rate exceeding 92%. Moreover, the adsorption process conformed to the quasi-second-order kinetic model and the Langmuir isothermal adsorption model, confirming the application potential of graphene oxide composite materials in the treatment of refractory organic wastewater.

2 Research on the Structural Characteristics and Adsorption Mechanism of Graphene Adsorbents

2.1 Research on Structural Regulation and Adsorption Active Sites

The adsorption performance of graphene-based materials depends on their structural regulation, mainly involving the synergistic effects of functional groups, defects, and pores. Graphene oxide (GO) is rich in functional groups such as hydroxyl and carboxyl, and the higher the density of functional groups, the stronger the adsorption capacity for heavy metals (such as the adsorption capacity for Pb^{2+} and Cu^{2+} can reach over 300 mg/g). Reduced graphene oxide (rGO) has reduced functional groups but restored conjugated structure, enhancing π-π interaction, and improving the adsorption capacity for aromatic pollutants by approximately 40%. Doped graphene (such as nitrogen and sulfur) introduces impurity atoms, optimizing adsorption selectivity. Additionally, increasing defect sites can enhance chemical adsorption capacity, and constructing mesoporous structures can improve mass transfer efficiency.

The synergistic effect of defect and pore structures is an important mechanism for enhancing the adsorption performance of graphene-based adsorbents. Defects in graphene sheets (such as edge defects and vacancy defects) can

serve as additional adsorption sites, cooperating with functional groups to capture pollutants; for example, for every 1% increase in the defect density of nitrogen-doped graphene, the adsorption capacity for methylene blue can increase by 8% [1]. Optimizing the pore structure (such as increasing the mesoporous proportion from 20% to 50%) can shorten the diffusion path of pollutants, increasing the adsorption rate constant by approximately 2 times. The essence of structural regulation lies in changing the electronic and spatial structure of graphene-based materials, thereby achieving precise design of active sites, providing a theoretical basis for the development of efficient water treatment adsorbents.

Future research on structural regulation should focus on multi-dimensional collaborative design, comprehensively applying strategies such as functional group modification, defect introduction, and pore optimization, to develop graphene-based adsorbents with high adsorption capacity, high selectivity, and rapid kinetics, thereby providing technical support for their practical water treatment applications.

2.2 A Literature Review on the Adsorption Mechanism of Typical Pollutants

For different pollutants, the adsorption mechanisms on the surface of graphene exhibit significant differences: for heavy metal ions, it is mainly chemical adsorption, with oxygen functional groups (such as hydroxyl and carboxyl) forming coordination bonds and electrostatic attraction playing a supplementary role. For organic dyes, physical adsorption and electrostatic interaction work together, and the large specific surface area provides physical sites, while the surface charge interacts with the charged groups of the dyes. For antibiotics, the mechanism is more complex, involving hydrogen bonds, π - π stacking, and electrostatic interactions, and the dominant mechanism varies with the structure of the antibiotic functional groups. The structural characteristics of graphene-based materials have a significant regulatory effect on the adsorption mechanism of pollutants. The original graphene has fewer surface functional groups, resulting in limited adsorption capacity for polar pollutants. While graphene oxide introduces a large number of oxygen functional groups, not only does it enhance the chemical interaction with polar pollutants, but also further optimizes the adsorption performance through structural modification. For example, the composite structure of graphene oxide/carbon nanotubes can utilize the supporting effect of carbon nanotubes to maintain the layer spacing of graphene oxide and avoid aggregation, thereby exposing more active adsorption sites, and the synergistic effect of the two materials can strengthen the adaptability of the adsorption mechanism to different types of pollutants[2].

The conclusions of the adsorption mechanisms of typical pollutants in different studies vary, mainly due to the differences in the preparation process of graphene materials, the degree of surface modification, the initial concentration of pollutants, and the pH of the solution, etc. For example, some studies suggest that heavy metal ions are mainly physical adsorption, which may be related to the low oxidation degree of graphene and insufficient surface functional groups; while in the adsorption of organic dyes, the primary and secondary relationship between electrostatic interaction and π-π stacking is controversial due to the differences in the conjugated structure of the dye molecules. These differences indicate that when studying the removal mechanism of graphene adsorbents, it is necessary to systematically consider the coupling effect of material structure and experimental conditions, so as to more accurately reveal their essence.

3 Research Progress on Performance Optimization of Graphene Adsorbents

3.1 The Mechanism by Which The Modification Strategy Enhances the Adsorption Performance

Improving the adsorption performance of graphene is a key approach through doping modification. By introducing elements such as N, S, and P, the electronic structure and surface chemical properties of graphene can be adjusted. Specifically, N doping can generate active sites such as pyridine N and pyrrole N, thereby enhancing the electrostatic attraction and complexation of polar pollutants; S doping relies on functional groups such as thiols and thioethers to improve the chelation effect on heavy metal ions; and P doping utilizes the lone pair electrons of phosphorus atoms to effectively enhance the π-π stacking and hydrogen bonding between graphene and organic dyes. The effects of different dopant atoms vary significantly. For example, the adsorption capacity of N-doped graphene for tetracycline in water can reach 120 mg/g, while the adsorption capacity of Pb^{2+} by S-doped graphene can be increased to over 250 mg/g[3].

Composite modification is an important way to expand the application scenarios of graphene adsorption. Combining with materials such as MOFs and biochar can achieve performance complementarity. The differences in the effects of different modification strategies stem from the different directions of regulating the adsorption mechanism of graphene: doping modification mainly optimizes the electronic structure and surface active sites, composite modification focuses on improving the mass transfer efficiency and adsorption capacity, and functional modification strengthens the selective adsorption ability. In practical applications, the appropriate modification method should be selected based on the properties of the target pollutants. For example, when treating heavy metal wastewater, S doping or functional modification should be preferred, and when treating organic pollutants, N doping or MOFs composite strategy can be adopted[3].

4 Research Summary and Future Prospects

4.1 Current Research Findings and Limitations

Research has shown that graphene adsorbents, with their two-dimensional sheet structure and abundant surface functional groups, can efficiently remove typical pollutants such as organic dyes and heavy metal ions from water through various mechanisms such as π - π stacking, hydrogen bonding, and electrostatic attraction. For instance, introducing functional groups such as hydroxyl and carboxyl through structural regulation can significantly enhance the selectivity of adsorption for specific pollutants. Moreover, the composite modification strategy (such as organic silicon composite graphene aerogel) further expands its application scenarios in the treatment of high-concentration and complex-component wastewater[4]. Additionally, the construction of adsorption kinetics and thermodynamics models provides theoretical support for predicting the adsorption process and optimizing process parameters. Some studies have achieved a removal rate of nearly 100% for pollutants in simulated wastewater, demonstrating the technical potential of graphene adsorbents.

Current research indicates that there is still a gap between theory and application for graphene adsorbents. Although there have been advancements in modification and modeling, due to the lack of systematic mechanism research and insufficient practical data, their engineering implementation remains challenging. In the future, it is necessary to integrate the synergistic adsorption mechanisms of multiple pollutants and rely on pilot-scale experiments to accumulate key data to promote large-scale applications.

4.2 Suggestions for Future Research Directions

Developing green and low-cost production processes is a crucial guarantee for promoting the large-scale application of graphene adsorbents. Traditional methods for preparing graphene mostly rely on chemical vapor deposition or redox methods, which have problems such as high energy consumption, large amounts of reagent pollution, and high costs, making it difficult to meet engineering requirements. In his research, Zhang Qiumo used biomass charcoal as a template and carbon source to prepare graphene-based composite aerogels through a one-step hydrothermal method. This not only reduced the production cost by approximately 40% but also reduced the use of chemical reagents, achieving the greenification of the material preparation process[5]. In the future, it is necessary to further explore the preparation paths using agricultural waste and industrial by-products as raw materials, combined with continuous production technology, to promote the reduction of the cost of graphene adsorbents and their large-scale production, laying the foundation for their wide application in water treatment fields.

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